

On Tree Representations of Relations and Graphs

Symbolic Ultrametrics and Cograph Edge Decompositions

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Received: date / Accepted: date

Abstract Tree representations of (sets of) symmetric binary relations, or equivalently edge-colored undirected graphs, are of central interest, e.g. in phylogenomics. In this context symbolic ultrametrics play a crucial role. Symbolic ultrametrics define an edge-colored complete graph that allows to represent the topology of this graph as a vertex-colored tree. Here, we are interested in the structure and the complexity of certain combinatorial problems resulting from considerations based on symbolic ultrametrics, and on algorithms to solve them.

This includes, the characterization of symbolic ultrametrics that additionally distinguishes between edges and non-edges of *arbitrary* edge-colored graphs G and thus, yielding a tree representation of G , by means of so-called cographs. Moreover, we address the problem of finding “closest” symbolic ultrametrics and show the NP-completeness of the three problems: symbolic ultrametric editing, completion and deletion. Finally, as not all graphs are cographs, and hence, don’t have a tree representation, we ask, furthermore, what is the minimum number of cotrees needed to represent the topology of an arbitrary non-cograph G . This is equivalent to find an optimal cograph

Parts of this paper were presented at the 21st Annual International Computing and Combinatorics Conference (COCOON 2015), August 4-6, 2015, Beijing, China [18]. This work was funded by the German Research Foundation (DFG) (Proj. No. MI439/14-1).

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edge k -decomposition $\{E_1, \dots, E_k\}$ of E so that each subgraph (V, E_i) of G is a cograph. We investigate this problem in full detail, resulting in several new open problems, and NP-hardness results.

For all optimization problems proven to be NP-hard we will provide integer linear program (ILP) formulations to efficiently solve them.

Keywords Symbolic Ultrametric · Cograph · Edge Partition · Editing · Integer Linear Program (ILP) · NP-complete

1 Introduction

Tree representations of relations between certain objects lie at the heart of many problems, in particular, in phylogenomic studies [15, 17, 20]. Phylogenetic Reconstructions are concerned with the study of the evolutionary history of groups of systematic biological units, e.g. genes or species. The objective is the assembling of so-called phylogenetic trees or networks that represent a hypothesis about the evolutionary ancestry of a set of genes, species or other taxa.

Consider a symmetric map $\delta: V \times V \rightarrow M^\odot$ that assigns to each pair (x, y) a symbol or color $m \in M^\odot$. The question then arises whether it is possible to determine a rooted tree T with a vertex-labeling t so that the lowest common ancestor $\text{lca}(x, y)$ of distinct leaves x and y in T is labeled with $m \in M^\odot$ if and only if $\delta(x, y) = m$. Such a tree is then called *symbolic representation* of δ . In phylogenomics, such maps δ can be interpreted as an assignment of evolutionary relationships between two genes and the symbolic representation of such relations then reflect the evolutionary history together with the respective events that happened when two genes diverged. It has recently been shown, that in theory [19] and in practice [17] it is even possible to reconstruct the evolutionary history of species, where the genes have been taken from, whenever the symbolic representation is known.

The problem of finding such symbolic representations (T, t) has been first addressed by Böcker and Dress [4] in a mathematical context. The authors showed, that there is a symbolic representation (T, t) of δ if and only if the map δ fulfills the properties of a so-called symbolic ultrametric [4]. Clearly, any such map $\delta: V \times V \rightarrow M^\odot$ is equivalent to a set of disjoint symmetric binary relations $\{R_m \mid m \in M^\odot\}$ with $(x, y) \in R_{\delta(x, y)}$ or an edge-colored complete graph $K_{|V|} = (V, \binom{V}{2})$ so that each edge $[x, y]$ obtains the color $\delta(x, y) \in M^\odot$. In [15] a characterization of symbolic ultrametrics in graph theoretical terms have been given. It has been shown that there is a symbolic representation (T, t) of such an edge-colored graph $K_{|V|}$ if the edges of each cycle of length 3 have at most two colors and each mono-chromatic subgraph G_m , i.e., subgraphs that consist of all the edges having a fixed color m , are so-called cographs. Cographs are characterized by the absence of induced paths P_4 on four vertices, although there are a number of equivalent characterizations of cographs (see e.g. [6] for a survey). Moreover, Lerchs [23, 24] showed that

each cograph $G = (V, E)$ is associated with a unique rooted tree $T(G)$, called *cotree*.

In this contribution we address several combinatorial problems that are concerned with symbolic ultrametrics and tree representations of arbitrary, possibly edge-colored graphs.

We first investigate in Section 3, under what conditions it is possible to find a symbolic ultrametric for arbitrary graphs G so that edges and non-edges of G can be distinguished. In other words, we ask for an edge-coloring of G so that edges and non-edges always obtain different colors and this coloring satisfies the conditions of a symbolic ultrametric. If such a coloring is known for G , then one can immediately display the topology of G as a tree via a symbolic representation (T, t) . It does not come as a big surprise, when we prove that such a symbolic ultrametric can only be defined for G if and only if G is already a cograph. This, in particular, establishes another new characterization of cographs. As a consequence we can infer that any symbolic representation (T, t) of a cograph G is a so-called refinement of its cotree.

In practice, however, symmetric maps $d: V \times V \rightarrow M^\odot$ represent often only estimates of the true relationship δ between the investigated objects, e.g., genes [21, 22]. Thus, in general such estimates d will not be a symbolic ultrametric. Hence, there is a great interest in optimally editing d to a symbolic ultrametric δ , i.e., finding a minimum number of changes of the assignment $d(x, y) \in M^\odot$ to pairs (x, y) so that there is a symbolic representation of the resulting map δ [17]. So far, the complexity of this problem has been unknown. In Section 4, we show that (the decision version of) this problem, called SYMBOLIC ULTRAMETRIC EDITING, is NP-complete. Additionally, we show that the problems SYMBOLIC ULTRAMETRIC COMPLETION and SYMBOLIC ULTRAMETRIC DELETION are NP-complete and provide integer linear program (ILP) formulations in order to efficiently solve the latter three problems in future work.

A further combinatorial problem we consider in Section 5 is motivated by the results established in Section 3 where we have characterized graphs for which one can find symbolic representations by means of cographs. However, not all graphs are cographs and thus, don't have such a tree representation. Therefore, we ask for the minimum number of cotrees that are needed to represent the structure of a given graph $G = (V, E)$ in an unambiguous way. As it will turn out, this problem is equivalent to find a decomposition $\Pi = \{E_1, \dots, E_k\}$ of E (i.e., the elements of Π need not necessarily be disjoint) for the least integer k , so that each subgraph $G_i = (V, E_i)$, $1 \leq i \leq k$ is a cograph. Such a decomposition is called cograph edge k -decomposition, or cograph k -decomposition, for short. If the elements of Π are in addition pairwise disjoint, we call Π a cograph k -partition. We show that the number of such optimal cograph k -decomposition, resp., partitions on a graph can grow exponentially in the number of vertices. Moreover, non-trivial upper bounds for the integer k such that there is a cograph k -decomposition, resp., partition are derived and polynomial-time algorithms to compute Π with $|\Pi| \leq \Delta + 1$, where Δ denotes the maximum number of edges a vertex is contained in, are provided.

Furthermore, we will prove that finding the least integer $k \geq 2$ so that G has a cograph k -decomposition or a cograph k -partition is an NP-hard problem. In order to attack this problem in future work, we derive ILP formulations to solve this problem efficiently. These findings complement results known about so-called cograph vertex partitions [1, 13, 10, 33].

2 Essential Definitions

Graph. In what follows, we consider undirected simple graphs $G = (V, E)$ with vertex set $V(G) = V$ and edge set $E(G) = E \subseteq \binom{V}{2}$. The *complement graph* $G^c = (V, E^c)$ of $G = (V, E)$, has edge set $E^c = \binom{V}{2} \setminus E$. The graph $K_{|V|} = (V, E)$ with $E = \binom{V}{2}$ is called *complete graph*. A graph $H = (W, F)$ is an *induced subgraph* of $G = (V, E)$, if $W \subseteq V$ and all edges $[x, y] \in E$ with $x, y \in W$ are contained in F . The *degree* $\deg(v) = |\{e \in E \mid v \in e\}|$ of a vertex $v \in V$ is defined as the number of edges that contain v . The maximum degree of a graph is denoted with Δ .

Rooted Tree. A connected graph T is a *tree*, if T does not contain cycles. A vertex of a tree T of degree one is called a *leaf* of T and all other vertices of T are called *inner* vertices. The set of inner vertices of T is denoted by V^0 and with E^0 we denote the set of *inner* edges, that are the edges in E where both of its end vertices are inner vertices. A *rooted tree* $T = (V, E)$ is a tree that contains a distinguished vertex $\rho_T \in V$ called the *root*. The first inner vertex $\text{lca}_T(x, y)$ that lies on both unique paths from distinct leaves x , resp., y to the root, is called *lowest common ancestor of x and y* . If there is no danger of ambiguity, we will write $\text{lca}(x, y)$ rather than $\text{lca}_T(x, y)$.

Symbolic Ultrametric and Symbolic Representation. In what follows, the set M will always denote a non-empty finite set, the symbol \odot will always denote a special element not contained in M , and $M^\odot := M \cup \{\odot\}$. Now, suppose X is an arbitrary non-empty set and $\delta : X \times X \rightarrow M^\odot$ a map. We call δ a *symbolic ultrametric* if it satisfies the following conditions:

- (U0) $\delta(x, y) = \odot$ if and only if $x = y$;
- (U1) $\delta(x, y) = \delta(y, x)$ for all $x, y \in X$, i.e. δ is symmetric;
- (U2) $|\{\delta(x, y), \delta(x, z), \delta(y, z)\}| \leq 2$ for all $x, y, z \in X$; and
- (U3) there exists no subset $\{x, y, u, v\} \in \binom{X}{4}$ such that $\delta(x, y) = \delta(y, u) = \delta(u, v) \neq \delta(y, v) = \delta(x, v) = \delta(x, u)$.

Now, suppose that $T = (V, E)$ is a rooted tree with leaf set X and that $t : V \rightarrow M^\odot$ is a map such that $t(x) = \odot$ for all $x \in X$. To the pair (T, t) we associate the map $d_{(T, t)}$ on $X \times X$ by setting, for all $x, y \in X$,

$$d_{(T, t)} : X \times X \rightarrow M^\odot; d_{(T, t)}(x, y) = t(\text{lca}_T(x, y)).$$

We call the pair (T, t) a *symbolic representation* of a map $\delta : X \times X \rightarrow M^\odot$, if $\delta(x, y) = d_{(T, t)}(x, y)$ holds for all $x, y \in X$. For a subset $W \subseteq X \times X$ we

denote with $\delta(W) = \{m \in M^\odot \mid \exists x, y \in W \text{ s.t. } \delta(x, y) = m\}$ the set of images of the elements contained in W .

We say that (T, t) and (T', t') are isomorphic if T and T' are isomorphic via a map $\varphi : V(T) \rightarrow V(T')$ such that $t'(\varphi(v)) = t(v)$ holds for all $v \in V(T)$.

Cographs and Cotrees. Complement-reducible graph, cographs for short, are defined as the class of graphs formed from a single vertex under the closure of the operations of union and complementation, namely: (i) a single-vertex graph is a cograph; (ii) the disjoint union of cographs is a cograph; (iii) the complement of a cograph is a cograph. Alternatively, a cograph can be defined as a P_4 -free graph (i.e. a graph such that no four vertices induce a subgraph that is a path of length 3). A number of equivalent characterizations of cographs can be found in [6]. It is well-known in the literature concerning cographs that, to any cograph $G = (V', E')$, one can associate a canonical *cotree* $T(G) = (V, E)$. This is a rooted tree, leaf set $V \setminus V^0$ equal to the vertex set V' of G and inner vertices that represent so-called "join" and "union" operations together with a labeling map $t : V^0 \rightarrow \{0, 1\}$ such $[x, y] \in E'$ if and only if $t(\text{lca}(x, y)) = 1$, and $t(v) \neq t(w_i)$ for all $v \in V^0$ and all children $w_1, \dots, w_k \in V^0$ of v , (cf. [9]). We will call the pair (T, t) *cotree representation* of G .

Cograph k -Decomposition and Partition, and Cotree Representation. Let $G = (V, E)$ be an arbitrary graph. A decomposition $\Pi = \{E_1, \dots, E_k\}$ of E is called (*cograph*) *k -decomposition*, if each subgraph $G_i = (V, E_i)$, $1 \leq i \leq k$ of G is a cograph. We call Π a (*cograph*) *k -partition* if $E_i \cap E_j = \emptyset$, for all distinct $i, j \in \{1, \dots, k\}$. A k -decomposition Π is called *optimal*, if Π has the least number k of elements among all cograph decompositions of G . Clearly, for a cograph only k -decompositions with $k = 1$ are optimal. A k -decomposition $\Pi = \{E_1, \dots, E_k\}$ is *coarsest*, if no elements of Π can be unified, so that the resulting decomposition is a cograph l -decomposition, with $l < k$. In other words, Π is coarsest, if for all subsets $I \subseteq \{1, \dots, k\}$ with $|I| > 1$ it holds that $(V, \cup_{i \in I} E_i)$ is not a cograph. Thus, every optimal k -decomposition is also always a coarsest one.

A graph $G = (V, E)$ is *represented by a set of cotrees* $\mathbb{T} = \{T_1, \dots, T_k\}$, each T_i with leaf set V , if and only if for each edge $[x, y] \in E$ there is a tree $T_i \in \mathbb{T}$ with $t(\text{lca}_{T_i}(x, y)) = 1$.

The Cartesian (Graph) Product $G \square H$ has vertex set $V(G \square H) = V(G) \times V(H)$; two vertices $(g_1, h_1), (g_2, h_2)$ are adjacent in $G \square H$ if $[g_1, g_2] \in E(G)$ and $h_1 = h_2$, or $[h_1, h_2] \in E(H)$ and $g_1 = g_2$. It is well-known that the Cartesian product is associative, commutative and that the single vertex graph K_1 serves as unit element [16, 14]. Thus, the product $\square_{i=1}^n G_i$ of arbitrary many factors G_1, \dots, G_n is well-defined. For a given product $\square_{i=1}^n G_i$, we define the G_i -layer G_i^w of G (through vertex w that has coordinates (w_1, \dots, w_n)) as the induced subgraph with vertex set $V(G_i^w) = \{v = (v_1, \dots, v_n) \in \times_{i=1}^n V(G_i) \mid v_j = w_j, \text{ for all } j \neq i\}$. Note, G_i^w is isomorphic to G_i for all $1 \leq i \leq n$, $w \in V(\square_{i=1}^n G_i)$. The *n -dimensional hypercube* Q_n or *n -cube*, for short, is the Cartesian product $\square_{i=1}^n K_2$.

3 Symbolic Ultrametrics and Cographs

Symbolic ultrametrics and respective representations as event-labeled trees, have been first characterized by Böcker and Dress [4].

Theorem 1 ([4, 15]) *Suppose $\delta : V \times V \rightarrow M^\odot$ is a map. Then there is a symbolic representation of δ if and only if δ is a symbolic ultrametric. Furthermore, this representation can be computed in polynomial time.*

Now, let $\delta : V \times V \rightarrow M^\odot$ be a map satisfying Properties (U0) and (U1). Clearly, the map δ can be considered as an edge coloring of a complete graph $K_{|V|}$, where each edge $[x, y]$ obtains color $\delta(x, y)$. For each fixed $m \in M$, we define the undirected graph $G_m := G_m(\delta) = (V, E_m)$ with edge set

$$E_m = \{[x, y] \mid \delta(x, y) = m, x, y \in V\}. \quad (1)$$

Hence, G_m denotes the subgraph of the edge-colored graph $K_{|V|}$, that contains all edges colored with $m \in M$. The following result establishes the connection between symbolic ultrametrics and cographs.

Theorem 2 ([15]) *Let $\delta : V \times V \rightarrow M^\odot$ be a map satisfying Properties (U0) and (U1). Then δ is a symbolic ultrametric if and only if*

- (U2') *For all $\{x, y, z\} \in \binom{V}{3}$ there is an $m \in M$ such that E_m contains (at least) two of the three edges $[x, y]$, $[x, z]$, and $[y, z]$. In other words, for each triangle induced by x, y and z , the edges have at most 2 different colors*
- (U3') *G_m is a cograph for all $m \in M$.*

Assume now, we have given an arbitrary none edge-colored graph $G = (V, E)$ and we want to represent the topology of G as a tree. The following question then arises:

Under which conditions is it possible to define an coloring on the edges and non-edges of G , so that edges $e \in E$ obtain a different color than the non-edges $e \in E^c$ of G and, in particular, so that the resulting map δ is a symbolic ultrametric?

In other words, we ask for an edge-coloring of G so that there is a tree (T, t) with $t(\text{lca}_T(x, y)) = m$ if and only if the (non)edge $[x, y]$ obtained color m and that edges and non-edges of G can be distinguished by this coloring, that is, edges and non-edges never obtain the same color. For an example of such an edge-colored graph G , see Figure 1. The following theorem gives necessary and sufficient conditions on the structure of graphs G for which one can find such a coloring and, in addition, provides a new characterization of cographs.

Theorem 3 *Let $G = (V, E)$ be an arbitrary (possibly disconnected) graph, $W = \{(x, y) \in V \times V \mid [x, y] \in E\}$ and $W^c = \{(x, y) \in V \times V \mid [x, y] \notin E\}$.*

There is a symbolic ultrametric $\delta : V \times V \rightarrow M^\odot$ s.t. $\delta(W) \cap \delta(W^c) = \emptyset$ if and only if G is a cograph.

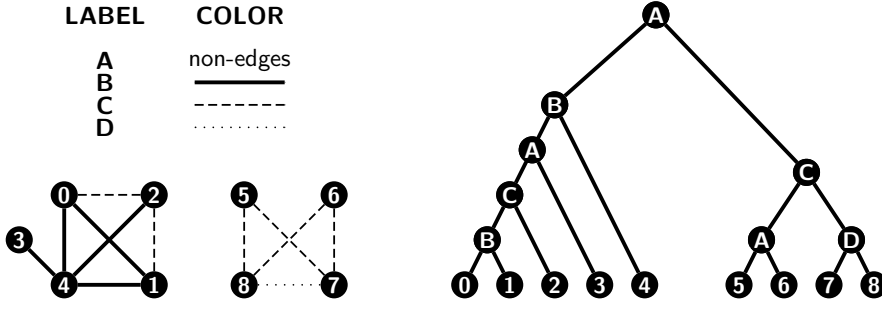


Fig. 1 Shown is a disconnected edge-colored graph G in the lower left part. The edge-colors are identified with the labels B , C and D , as indicated in the upper left part. Non-edges are identified with the label A . It is easy to verify that the event-labeled tree on the right hand side (T, t) is a tree representation of G , since for all distinct leaves i and j we have $\text{lca}_T(i, j) = X \in \{A, B, C, D\}$ if and only if the (non-)edge $[i, j]$ has the color identified with the respective label X .

In particular, G is a cograph and its cotree representation can be obtained by replacing the label A by 0, all other labels B, C, D by 1 and additional contraction of the interior edges $[C, B]$ and $[C, D]$.

Proof First assume that G is a cograph. Set $\delta(x, x) = \odot$ for all $x \in V$ and set $\delta(x, y) = \delta(y, x) = 1$ if $[x, y] \in E$ and, otherwise, to 0. Hence, condition (U0) and (U1) are fulfilled. Moreover, by construction $|M| = 2$ and thus, Condition (U2') is trivially fulfilled. Furthermore, since $G_1(\delta)$ and its complement $G_0(\delta)$ are cographs, (U3') is satisfied. Theorem 2 implies that δ is a symbolic ultrametric.

Now, let $\delta : V \times V \rightarrow M^\odot$ be a symbolic ultrametric with $\delta(W) \cap \delta(W^c) = \emptyset$. Assume for contradiction that G is not a cograph. Then G contains an induced path $P_4 = a - b - c - d$. Therefore, at least one edge e of this P_4 must obtain a color $\delta(e)$ different from the other two edges contained in this P_4 , as otherwise $G_{\delta(e)}(\delta)$ is not a cograph and thus, δ is not a symbolic ultrametric (Thm. 2, (U3')). For all such possible maps δ “subdividing” this P_4 we always obtain that two edges of at least one of the underlying paths $P_3 = a - b - c$ or $b - c - d$ must have different colors. W.l.o.g. assume that $\delta(a, b) \neq \delta(b, c)$. Since $[a, c] \notin E$ and $\delta(W) \cap \delta(W^c) = \emptyset$ we can conclude that $\delta(a, c) \neq \delta(a, b)$ and $\delta(a, c) \neq \delta(b, c)$. But then Condition (U2') cannot be satisfied, and Theorem 2 implies that δ is not a symbolic ultrametric. \square

Theorem 3 implies, that there is no hope for finding an edge-distinguishing map δ for a graph G , that assigns symbols or colors to edges, resp., non-edges such that for δ (and hence, for G) there is a symbolic representation (T, t) , unless G is already a cograph. However, this result does not come as a big surprise, as a cograph G is characterized by the existence of a unique (up to isomorphism) cotree (T', t') representing the topology of G . As a consequence of this result we can infer that any symbolic representation (T, t) of a cograph G is a refinement of the cotree representation (T', t') of G , that is, the cotree representation (T', t') of G can be obtained from the symbolic representation (T, t) of δ by the following procedure:

First reset for each $v \in V$,

$$t(v) = \begin{cases} \odot & \text{if } v \in V \setminus V^0, \text{ i.e., } v \text{ is a leaf} \\ 1 & \text{if } v = \text{lca}_T(x, y) \text{ and } \delta(x, y) \in W, \text{ i.e., } [x, y] \text{ is an edge in } G \\ 0 & \text{if else, i.e., } [x, y] \text{ is not an edge in } G \end{cases}$$

Clearly, this new map t on the tree T defines a symbolic representation (T, t) of the cograph $G = (V, E)$ so that $[x, y] \in E$ if and only if $t(\text{lca}_T(x, y)) = 1$. However, it might be possible that there is an edge $e = [u, v] \in E^0(T)$ such that $t(u) = t(v)$, and therefore, (T, t) is not a cotree representation. In this case, identify a new vertex v_e with e and define the tree $T_e = (V_e, E_e)$ with vertex set $V_e = V(T) \setminus \{u, v\} \cup \{v_e\}$, edge set $E_e = E(T) \setminus \{e\} \cup \{[v_e, w] : [w, u] \text{ or } [w, v] \in E\}$, that is again a rooted tree. Define for all $w \in V_e$ the map

$$t_e(w) = t(w) \text{ if } w \neq v_e \text{ and } t(v_e) = t(u). \quad (2)$$

This construction can be repeated, with (T_e, t_e) now playing the role of (T, t) , until we end in a rooted tree $\widehat{T} = (\widehat{V}, \widehat{E})$ with a map $\widehat{t} : \widehat{V} \rightarrow M^\odot$ so that for all edges $[u, v] \in \widehat{E}^0$ it holds that $\widehat{t}(u) \neq \widehat{t}(v)$.

With this procedure, we obtain a symbolic representation $(\widehat{T}, \widehat{t})$ of the cograph G , also known as so-called *discriminating* symbolic ultrametric [15]. In particular, this representation $(\widehat{T}, \widehat{t})$ is unique (up to isomorphism) [15, cf. Prop. 1] and, by construction, satisfies the condition of a cotree representation. Moreover, since the cotree representation (T', t') is unique (up to isomorphism) [23, 24], it follows that (T', t') and $(\widehat{T}, \widehat{t})$ must be isomorphic. We summarize this result in the following corollary.

Corollary 1 *Let $G = (V, E)$ be a cograph, (T', t') be the corresponding cotree representation, and W , resp., W^c as defined in Theorem 3. Moreover, assume that there is a symbolic ultrametric $\delta : V \times V \rightarrow M^\odot$ s.t. $\delta(W) \cap \delta(W^c) = \emptyset$ with (T, t) being the corresponding symbolic representation of δ .*

Assume that the pair $(\widehat{T}, \widehat{t})$ is obtained from (T, t) by application of the procedure above. Then, $(\widehat{T}, \widehat{t})$ and (T', t') are isomorphic.

Assume that we want to find a symbolic ultrametric that can distinguish between “most of” the edges and/or non-edges, however, the given graph is a non-cograph $G = (V, E)$. Then, we are immediately left with the following problems.

Problem COGRAPH EDITING/DELETION/COMPLETION

Input: Given a simple graph $G = (V, E)$ and an integer k .
Question: Is there a cograph $G' = (V, E')$, s.t.
 $E' \subseteq \binom{V}{2}$ and $|E \Delta E'| \leq k$ (Editing),
 $E' \subseteq E$ and $|E \setminus E'| \leq k$ (Deletion), or
 $E \subseteq E'$ and $|E' \setminus E| \leq k$ (Completion).

However, the (decision version of the) problem to edit a given graph G into a cograph G' , and thus, to find the closest graph G' that has a symbolic representation, is NP-complete [25,26]. In addition, the problems of deciding whether there is a cograph G' resulting by adding, resp., removing k edges from G is NP-complete, as well [11].

Theorem 4 (Liu et al. [26], El-Mallah and Colbourn [11]) COGRAPH EDITING, COGRAPH COMPLETION and COGRAPH DELETION are NP-complete.

In what follows, we will consider and discuss two modifications of the problem of finding a symbolic ultrametric that can distinguish between edges and non-edges in Section 4 and 5:

1. In Section 4 we consider a couple of problems which are of highly practical relevance: The symbolic ultrametric editing, completion and deletion problem.
2. In contrast, if a non-edge colored graph G is not a cograph and thus, if there is no single tree representation of G , then we ask for the minimum number of trees that are needed in order to represent the topology of G in an unambiguous way, see Section 5.

4 Symbolic Ultrametric Editing, Completion and Deletion

Symbolic ultrametrics lie at the heart of many problems in phylogenomics. Phylogenetic Reconstructions are concerned with the study of the evolutionary history of groups of systematic biological units, e.g. genes or species. The objective is the assembling of so-called phylogenetic trees or networks that represent a hypothesis about the evolutionary ancestry of a set of genes, species or other taxa.

Genes are passed from generation to generation to the offspring. Some of those genes are frequently duplicated, mutate or get lost - a mechanism that also ensures that new species can evolve. Crucial for the evolutionary reconstruction of species history is the knowledge of the relationship between the respective genes. Genes that share a common origin (homologs) are divided into three classes, namely orthologs, paralogs, and xenologs [12]. Two homologous genes are orthologous if at their most recent point of origin the ancestral gene complement is transmitted to two daughter lineages; a speciation event happened. They are paralogous if the ancestor gene at their most recent point of origin was duplicated within a single ancestral genome; a duplication event happened. Horizontal gene transfer (HGT) refers to the transfer of genes between organisms in a manner other than traditional reproduction and across different species; if such an event happened at the most recent point of origin of two genes, then they are called xenologous. Intriguingly, there are practical sequence-based methods that allow to determine whether two genes x and y are orthologs or not with acceptable accuracy *without* constructing either gene or species trees [21,22].

Now, assume we have given an estimate of genes being orthologs, paralogs or even xenologs, that is a map $d : X \times X \rightarrow \{\text{speciation, duplication, HGT}\}$. Then, one is interested in the representation of these estimates as a tree T with event-labeling t so that $t(\text{lca}(x, y)) = \text{speciation}$ iff x, y are orthologs, $t(\text{lca}(x, y)) = \text{duplication}$ iff x, y are paralogs and $t(\text{lca}(x, y)) = \text{HGT}$ iff x, y are xenologs. In practice, however, such maps d are often only estimates of the true evolutionary relationship δ between the investigated genes. Thus, in general such estimates d will not be a symbolic ultrametric. Hence, there is a big interest in optimally editing d to a symbolic ultrametric δ .

The problem of editing a given symmetric map $d : X \times X \rightarrow M^\odot$ to a symbolic ultrametric is defined as follows:

Problem SYMBOLIC ULTRAMETRIC EDITING

- Input:* Given a symmetric map $d : X \times X \rightarrow M^\odot$, s.t.
 $d(x, y) = \odot$ if and only if $x = y$.
- Question:* Is there a symbolic ultrametric $\delta : X \times X \rightarrow M^\odot$, s.t. for
 $D = \{(x, y) \in X \times X \mid d(x, y) \neq \delta(x, y)\}$ we have $|D| \leq k$.

A further problem arising from the latter considerations is as follows. Assume we have an assignment of a symmetric subset R of $X \times X$ so that for all $(x, y) \in R$ the assignment $d(x, y)$ is believed to be a reliable estimate and thus, which is not allowed to be changed. Moreover, let $X \times X \setminus R$ be the pairs (x, y) for which an assignment $d(x, y)$ is not known. Assume that $M = \{1, \dots, n\}$ and $M^\odot = M \cup \{\odot, 0\}$, then we can extend the map $d : X \times X \rightarrow M^\odot$ so that

$$d(x, y) = \begin{cases} \odot & \text{if } x = y \\ d(x, y) & \text{if } (x, y) \in R \\ 0 & \text{if } (x, y) \in X \times X \setminus R \end{cases}$$

We then ask to change the assignment of a minimum number of pairs (x, y) with $d(x, y) = 0$ to some element in $m \in M, m \neq 0$ so that the resulting map is a symbolic ultrametric. In other words, only non-reliable estimates of pairs (x, y) are allowed to be changed.

Problem SYMBOLIC ULTRAMETRIC COMPLETION

- Input:* Given a symmetric map $d : X \times X \rightarrow M^\odot$, s.t.
 $d(x, y) = \odot$ if and only if $x = y$.
- Question:* Is there a symbolic ultrametric $\delta : X \times X \rightarrow M^\odot$ s.t.
if $d(x, y) \neq 0$, then $\delta(x, y) = d(x, y)$; and $|D| \leq k$, where
 $D = \{(x, y) \in X \times X \mid d(x, y) \neq \delta(x, y)\}$.

Conversely, one might ask to change a minimum number of assignments $d(x, y) \neq 0$ to $\delta(x, y) = 0$.

Problem SYMBOLIC ULTRAMETRIC DELETION

- Input:* Given a symmetric map $d : X \times X \rightarrow M^\odot$, s.t.
 $d(x, y) = \odot$ if and only if $x = y$.
- Question:* Is there a symbolic ultrametric $\delta : X \times X \rightarrow M^\odot$ s.t.
 $\delta(x, y) = d(x, y)$ or $\delta(x, y) = 0$; and $|D| \leq k$, where
 $D = \{(x, y) \in X \times X \mid d(x, y) \neq \delta(x, y)\}$.

4.1 Computational Complexity

In this section, we prove the NP-completeness of SYMBOLIC ULTRAMETRIC EDITING, SYMBOLIC ULTRAMETRIC COMPLETION and SYMBOLIC ULTRAMETRIC DELETION.

Theorem 5 SYMBOLIC ULTRAMETRIC EDITING is NP-complete.

Proof Given a symmetric map δ it can be verified in polynomial time, if δ is a symbolic ultrametric: One can check Conditions (U2) and (U3) individually for each of the $O(|X|^3)$ many combinations of $\{x, y, z\} \in \binom{X}{3}$ for (U2), and the $O(|X|^4)$ many combinations of $\{x, y, u, v\} \in \binom{X}{4}$ for (U3), respectively. Hence, SYMBOLIC ULTRAMETRIC EDITING \in NP. We will show by reduction from COGRAPH EDITING that SYMBOLIC ULTRAMETRIC EDITING is NP-hard.

Let $G = (V, E)$ be an arbitrary simple graph. We associate with G a map $d: V \times V \rightarrow M^\odot$, where $M = \{0, 1, \dots, n\}$ is a non-empty finite set s.t. $n \geq 1$ and thus, $0, 1 \in M$. Let $M^\odot := M \cup \{\odot\}$ and set for all $x, y \in V$:

$$d(x, y) = d(y, x) = \begin{cases} \odot & \text{if } x = y \\ 1 & \text{if } [x, y] \in E \\ 0 & \text{if } [x, y] \notin E \end{cases}$$

Obviously, d can be constructed in polynomial time. In the following, we show, that given an integer k , there exists a solution of the COGRAPH EDITING problem for G and integer k if and only if there exists a solution of the SYMBOLIC ULTRAMETRIC EDITING problem for d and integer $2k$.

First, we show that a solution of the SYMBOLIC ULTRAMETRIC EDITING problem for d and $2k$ can be constructed from a solution of the COGRAPH EDITING problem for G and k . Let $G' = (V, E')$ be a cograph with $|E \Delta E'| \leq k$. Furthermore let $\delta: V \times V \rightarrow M^\odot$ be a map, such that for all $x, y \in V$,

$$\delta(x, y) = \delta(y, x) = \begin{cases} \odot & \text{if } x = y \\ 1 & \text{if } [x, y] \in E' \\ 0 & \text{if } [x, y] \notin E' \end{cases}$$

It is easy to verify that δ is a symbolic ultrametric by application of Theorem 2. It remains to show that for $D = \{(x, y) \in X \times X \mid d(x, y) \neq \delta(x, y)\}$ it holds that $|D| \leq 2k$. Note that for all $x \in V$ we have $d(x, x) = \delta(x, x) = \odot$ and therefore $(x, x) \notin D$. The set D can be partitioned into the two subsets

$$\begin{aligned} D_1 &= \{(x, y) \mid d(x, y) = 1 \wedge \delta(x, y) = 0\} \text{ and} \\ D_2 &= \{(x, y) \mid d(x, y) = 0 \wedge \delta(x, y) = 1\}. \end{aligned}$$

Hence, $(x, y) \in D_1$ if and only if $[x, y] \in E \setminus E'$, and $(x, y) \in D_2$ if and only if $[x, y] \in E' \setminus E$. As $(E \setminus E') \cup (E' \setminus E) = (E \Delta E')$ it holds that, $(x, y) \in D$ if and only if $[x, y] \in E \Delta E'$. As d and δ are symmetric, it also holds that $(x, y) \in D$ if and only if $(y, x) \in D$. Hence, $[x, y] \in E \Delta E'$ if and only if $(x, y) \in D$

and $(y, x) \in D$. This reflects the fact, that an edge edit $[x, y] \in E\Delta E'$ in G corresponds to the two symmetric edits $(x, y), (y, x) \in D$ in d . Therefore, $|D| = |\{(x, y) \mid d(x, y) \neq \delta(x, y)\}| = 2|E\Delta E'| \leq 2k$.

We continue to show that a solution of the COGRAPH EDITING problem for G and k can be constructed from a solution of the SYMBOLIC ULTRAMETRIC EDITING problem for d and $2k$. Let $\delta : V \times V \rightarrow \widetilde{M}^\odot$ be a symbolic ultrametric s.t. $|D| = |\{(x, y) \mid d(x, y) \neq \delta(x, y)\}| \leq 2k$. Furthermore, let $G' = (V, E')$ be a simple graph, such that for all $x, y \in V$ it holds that $[x, y] \in E'$ if and only if $\delta(x, y) = 1$. By Theorem 2 (U3') we have that $G' = G_1$ and hence, G' is a cograph. It remains to show that $|E\Delta E'| \leq k$. By construction, for all $x \in V$, $d(x, x) = \delta(x, x) = \odot$ and $[x, x] \notin E\Delta E'$. Let $D = \{(x, y) \mid d(x, y) \neq \delta(x, y)\}$. Note that for all distinct $x, y \in V$ it holds that $d(x, y) \in \{0, 1\}$. Hence, D can be partitioned into the four subsets

$$\begin{aligned} D_1 &= \{(x, y) \mid d(x, y) = 1 \wedge \delta(x, y) = 0\}, \\ D_2 &= \{(x, y) \mid d(x, y) = 0 \wedge \delta(x, y) = 1\}, \\ D_3 &= \{(x, y) \mid d(x, y) = 1 \wedge \delta(x, y) \in \widetilde{M}^\odot \setminus \{0, 1\}\}, \text{ and} \\ D_4 &= \{(x, y) \mid d(x, y) = 0 \wedge \delta(x, y) \in \widetilde{M}^\odot \setminus \{0, 1\}\}. \end{aligned}$$

For these subsets of D it holds that if $(x, y) \in D_1$ then $[x, y] \in E \setminus E'$, and if $(x, y) \in D_2$ then $[x, y] \in E' \setminus E$. Furthermore, $\delta(x, y) \in \widetilde{M}^\odot \setminus \{0, 1\}$ implies that $[x, y] \notin E'$ and it follows that if $(x, y) \in D_3$ then $[x, y] \in E \setminus E'$, and if $(x, y) \in D_4$ then $[x, y] \notin E \wedge [x, y] \notin E'$. For all remaining $x, y \in V$, i.e., for which $d(x, y) = \delta(x, y)$, it holds that $[x, y] \notin E \setminus E'$ and $[x, y] \notin E' \setminus E$. It follows that $[x, y] \in E \setminus E'$ if and only if $(x, y) \in D_1 \cup D_3$, and $[x, y] \in E' \setminus E$ if and only if $(x, y) \in D_2$. As before, due to the symmetry of the maps d and δ , two symmetric edits $(x, y), (y, x) \in D$ in d correspond to at most one edge edit $[x, y] \in E\Delta E'$ in G . Finally, $2|E\Delta E'| = 2|E \setminus E'| + 2|E' \setminus E| = |D_1 \cup D_3| + |D_2| \leq |D| \leq 2k$. Hence, $|E\Delta E'| \leq k$.

Thus, SYMBOLIC ULTRAMETRIC EDITING is NP-complete. \square

Theorem 6 SYMBOLIC ULTRAMETRIC COMPLETION is NP-complete.

Proof It is shown analogously as in the proof of Theorem 5 that SYMBOLIC ULTRAMETRIC MIN COMPLETION $\in NP$. We will show by reduction from COGRAPH COMPLETION that SYMBOLIC ULTRAMETRIC COMPLETION is NP-hard.

Let $G = (V, E)$ be an arbitrary simple graph. We associate to G a map $d : V \times V \rightarrow M^\odot$ as defined in the proof of Theorem 5:

$$d(x, y) = d(y, x) = \begin{cases} \odot & \text{if } x = y \\ 1 & \text{if } [x, y] \in E \\ 0 & \text{if } [x, y] \notin E \end{cases}$$

Let there be a solution $G' = (V, E')$ for the COGRAPH COMPLETION problem for G and k , i.e., $E \subseteq E'$ and $|E' \setminus E| \leq k$. We show that there is

a solution for the SYMBOLIC ULTRAMETRIC COMPLETION problem for d and $2k$. Define the map $\delta: V \times V \rightarrow M^\odot$ as in the proof of Theorem 5:

$$\delta(x, y) = \delta(y, x) = \begin{cases} \odot & \text{if } x = y \\ 1 & \text{if } [x, y] \in E' \\ 0 & \text{if } [x, y] \notin E' \end{cases}$$

Again, it is easy to verify that δ is a symbolic ultrametric by application of Theorem 2. Moreover, by construction $\delta(x, y) = d(x, y)$ for all $x, y \in V$ whenever $[x, y] \in E \subseteq E'$ and hence, for all $x, y \in V$ with $d(x, y) \neq 0$.

It remains to show that for $D = \{(x, y) \in X \times X \mid 0 = d(x, y) \neq \delta(x, y)\}$ it holds that $|D| \leq 2k$. Note that for all $x \in V$ we have $d(x, x) = \delta(x, x) = \odot$ and therefore $(x, x) \notin D$. Moreover,

$$D = \{(x, y) \mid d(x, y) = 0 \wedge \delta(x, y) = 1\}.$$

Hence, $(x, y), (y, x) \in D$ if and only if $[x, y] \in E' \setminus E$. Therefore, $|D| = 2|E' \setminus E| \leq 2k$.

We continue to show that a solution of the COGRAPH EDITING problem for G and k can be constructed from a solution of the SYMBOLIC ULTRAMETRIC EDITING problem for d and $2k$. Let $\delta: V \times V \rightarrow \widetilde{M}^\odot$ be a symbolic ultrametric s.t. $|D| \leq 2k$ and $\delta(x, y) = d(x, y)$ if $d(x, y) \neq 0$. Furthermore, let $G' = (V, E')$ be a simple graph, such that for all $x, y \in V$ it holds that $[x, y] \in E'$ if and only if $\delta(x, y) = 1$. By Theorem 2 (U3') we have that $G' = G_1$ and hence, G' is a cograph. It remains to show that $|E' \setminus E| \leq k$. By construction, for all $x \in V$, $d(x, x) = \delta(x, x) = \odot$ and $[x, x] \notin E'$. Note that for all distinct $x, y \in V$ it holds for the map associated to G that $d(x, y) \in \{0, 1\}$. Hence, D can be partitioned into

$$\begin{aligned} D_1 &= \{(x, y) \mid d(x, y) = 0 \wedge \delta(x, y) = 1\}, \text{ and} \\ D_2 &= \{(x, y) \mid d(x, y) = 0 \wedge \delta(x, y) \in \widetilde{M}^\odot \setminus \{0, 1\}\}. \end{aligned}$$

Thus, if $(x, y), (y, x) \in D_1$, then $[x, y] \in E' \setminus E$. Therefore, $2(|E' \setminus E|) = |D_1| \leq |D| \leq 2k$ and thus, $|E' \setminus E| \leq k$.

Hence, SYMBOLIC ULTRAMETRIC COMPLETION is NP-complete. \square

Using similar arguments as in the proof of Theorem 6 we can infer the NP-completeness of SYMBOLIC ULTRAMETRIC DELETION by reduction from COGRAPH DELETION.

Theorem 7 SYMBOLIC ULTRAMETRIC DELETION is NP-complete.

4.2 Integer Linear Program

We showed in [17] that the cograph editing problem is amenable to formulations as Integer Linear Program (ILP). We will extend these results here to solve the symbolic ultrametric editing/completion/deletion problem. Let

$d : X \times X \rightarrow M^\odot$ be an arbitrary symmetric map with $M = \{0, 1, \dots, n\}$ and $K_{|X|} = (X, E = \binom{X}{2})$ be the corresponding complete graph with edge-coloring s.t. each edge $[x, y] \in E$ obtains color $d(x, y) = d(y, x)$.

For each of the three problems and hence, a given symmetric map d we define for each distinct $x, y \in X$ and $i \in M$ the binary constants $\mathfrak{d}_{x,y}^i$ with $\mathfrak{d}_{x,y}^i = 1$ if and only if $d(x, y) = i$. Moreover, we define the binary variables E_{xy}^i for all $i \in M$ and $x, y \in X$ that reflect the coloring of the edges in $K_{|V|}$ of the final symbolic ultrametric δ , i.e., E_{xy}^i is set to 1 if and only if $\delta(x, y) = i$.

In order to find the closest symbolic ultrametric δ , the objective function is to minimize the symmetric difference of the d and δ among all different symbols $i \in M$:

$$\min \sum_{i \in M} \left(\sum_{(x,y) \in X} (1 - \mathfrak{d}_{xy}^i) E_{xy}^i + \sum_{(x,y) \in X} \mathfrak{d}_{xy}^i (1 - E_{xy}^i) \right) \quad (3)$$

The same objective function can be used for the symbolic ultrametric completion and deletion problem.

In case of the the symbolic ultrametric completion we must ensure that $\delta(x, y) = d(x, y)$ for all $d(x, y) \neq 0$. Hence we set for all x, y with $d(x, y) = i \neq 0$:

$$E_{x,y}^i = 1. \quad (4)$$

In case of the symbolic ultrametric deletion we must ensure that $\delta(x, y) = d(x, y)$ or $\delta(x, y) = 0$ or, in other words, for all $d(x, y) = i \neq 0$ it must hold that either $E_{xy}^i = 1$ or $E_{xy}^0 = 1$. Hence, we set for for all for all $x, y \in V$:

$$E_{xy}^0 = 1, \text{ if } d(x, y) = 0, \text{ and } E_{xy}^i + E_{xy}^0 = 1, \text{ else.} \quad (4')$$

For the cograph editing problem we neither need Constraint 4 nor 4'. However, for all three problems we need the following.

Each tuple (x, y) with $x \neq y$ has exactly one value $i \in M$ assigned to it which is expressed in the following constraint.

$$\sum_{i \in M} E_{x,y}^i = 1 \text{ and } E_{xy}^i - E_{yx}^i = 0 \text{ for all } x, y \in X. \quad (5)$$

In order to satisfy Condition (U2') and thus, that all induced triangles have at most two colors on the edges we need this constraint.

$$E_{xy}^i + E_{yz}^j + E_{xz}^k \leq 2 \quad (6)$$

for all ordered tuples (i, j, k) of distinct $i, j, k \in M$ and pairwise distinct $x, y, z \in X$.

Finally, in order to satisfy Condition (U3') and thus, that each monochromatic subgraph comprising all edges with fixed color i is a cograph, we need the following constraint that forbids induced P_4 's.

$$E_{xy}^i + E_{yu}^i + E_{uv}^i - E_{xu}^i - E_{xv}^i - E_{yv}^i \leq 2 \quad (7)$$

for all $i \in M$ and all ordered tuples (x, y, u, v) of distinct $x, y, u, v \in X$.

It is easy to verify that the latter ILP formulation needs $O(|M||X|^2)$ variables and $O(|M|^3|X|^3 + |X|^4)$ constraints.

5 Cotree Representation and Cograph k -Decomposition

If a given non-edge colored graph G is not a cograph, then Theorem 3 implies that one cannot define an edge-distinguishing symbolic ultrametric, and thus, in particular no single tree representation of G . Therefore, we are interested to represent the topology of G in an unambiguous way with a minimum number of trees.

Recollect, a graph $G = (V, E)$ is represented by a set of cotrees $\mathbb{T} = \{T_1, \dots, T_k\}$, if and only if for each edge $[x, y] \in E$ there is a tree $T_i \in \mathbb{T}$ with $t(\text{lca}_{T_i}(x, y)) = 1$.

Note, by definition, each cotree T_i determines a subset $E_i = \{[x, y] \in E \mid t(\text{lca}_{T_i}(x, y)) = 1\}$ of E . Hence, the subgraph (V, E_i) of G must be a cograph. Therefore, in order to find the minimum number of cotrees representing a graph G , we can equivalently ask for a decomposition $\Pi = \{E_1, \dots, E_k\}$ of E so that each subgraph (V, E_i) is a cograph, where k is the least integer among all cograph decompositions of G . Thus, we are dealing with the following two equivalent problems.

Problem COTREE k -REPRESENTATION

Input: Given a graph $G = (V, E)$ and an integer k .

Question: Can G be represented by k cotrees?

Problem COGRAPH k -DECOMPOSITION

Input: Given a graph $G = (V, E)$ and an integer k .

Question: Is there a cograph k -decomposition of G ?

Clearly, any cograph has an optimal 1-decomposition, while for cycles of length > 4 or paths P_4 there is always an optimal cograph 2-decomposition. However, there are examples of graphs that even do not have a cograph 2-decomposition, see Figure 2. Moreover, as shown in Figure 3, the number of different optimal cograph k -decomposition on a graph can grow exponentially. the next theorem provides a non-trivial upper bound for the integer k s.t. there is still a cograph k -decomposition for arbitrary graphs.

Theorem 8 *For every graph G with maximum degree Δ there is a cograph k -decomposition with $1 \leq k \leq \Delta + 1$ that can be computed in $O(|V||E| + \Delta(|V| + |E|))$ time. Hence, any graph can be represented by at most $\Delta + 1$ cotrees.*

Proof Consider a proper edge-coloring $\varphi : E \rightarrow \{1, \dots, k\}$ of G , i.e., an edge coloring such that no two incident edges obtain the same color. Any proper edge-coloring using k colors yields a cograph k -partition $\Pi = \{E_1, \dots, E_k\}$ where $E_i = \{e \in E \mid \varphi(e) = i\}$, because any connected component in $G_i = (V, E_i)$ is an edge and thus, no P_4 's are contained in G_i . Vizing's Theorem [32]

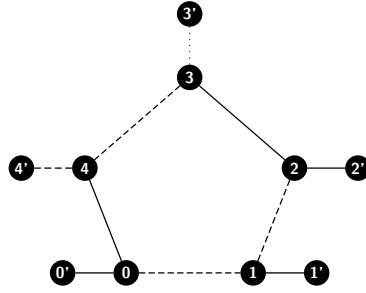


Fig. 2 Full enumeration of all possibilities (which we leave to the reader), shows that the depicted graph has no cograph 2-decomposition. The existing cograph 3-decomposition is also a cograph 3-partition; highlighted by dashed-lined, dotted and bold edges.

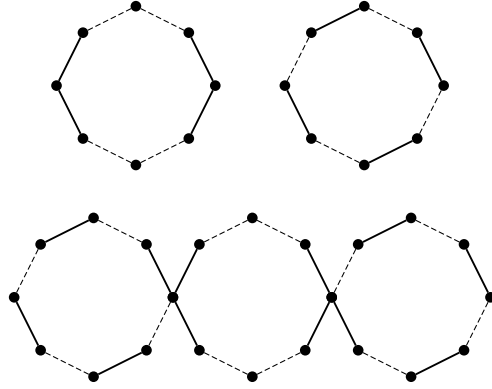


Fig. 3 Two isomorphic graphs with two non-equivalent optimal cograph 2-decomposition (highlighted by dashed and solid edges) are shown in the upper part. By stepwisely identifying single vertices one obtains a chain of graphs G , see lower part. For each subgraph that is a copy of the graph above, an optimal cograph 2-decomposition can be determined almost independently of the remaining parts of the graph G . Hence, with an increasing number of vertices of such chains G the number of different cograph 2-decompositions is growing exponentially.

implies that for each graph there is a proper edge-coloring using k colors with $\Delta \leq k \leq \Delta + 1$.

An proper edge-coloring using at most $\Delta + 1$ colors can be computed with the Misra-Gries-algorithm in $O(|V||E|)$ time [27]. Since the (at most $\Delta + 1$) respective cotrees can be constructed in linear-time $O(|V| + |E|)$ [8], we derive the runtime $O(|V||E| + \Delta(|V| + |E|))$. \square

Obviously, any optimal k -decomposition must also be a coarsest k -decomposition, while the converse is in general not true, see Fig. 4. The partition $\Pi = \{E_1, \dots, E_k\}$ obtained from a proper edge-coloring is usually not a coarsest one, as possibly (V, E_J) is a cograph, where $E_J = \cup_{i \in J} E_i$ and $J \subseteq \{1, \dots, k\}$. However, there are graphs having an *optimal* cograph Δ -decomposition, see Fig. 2 and 3. Thus, the derived bound $\Delta + 1$ is almost sharp. Nevertheless, we assume that this bound can be sharpened:

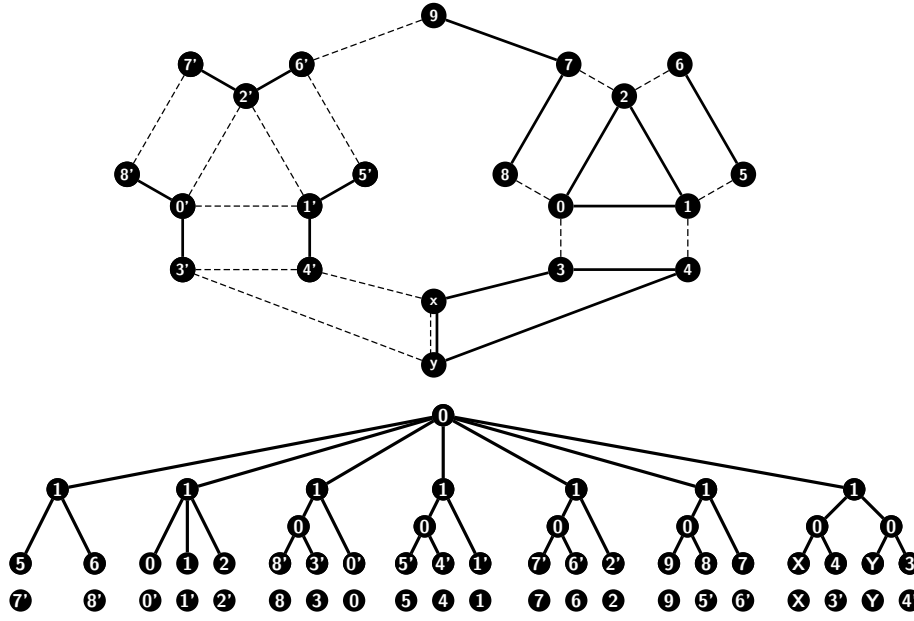


Fig. 4 The shown (non-co)graph G has a 2-decomposition $\Pi = \{E_1, E_2\}$. Edges in the different elements E_1 and E_2 are highlighted by dashed and solid edges, respectively. Thus, two cotrees, shown in the lower part of this picture, are sufficient to represent the structure of G . The two cotrees are isomorphic, and thus, differ only in the arrangement of their leaf sets. For this reason, we only depicted one cotree with two different leaf sets. Note, G has no 2-partition, but a coarsest 3-partition. The latter can easily be verified by application of the construction in Lemma 1.

Conjecture 1 For every graph G with maximum degree Δ there is a cograph Δ -decomposition.

However, there are examples of non-cographs containing many induced P_4 's that have a cograph k -decomposition with $k \ll \Delta + 1$, which implies that any optimal k -decomposition of those graphs will have significantly less elements than $\Delta + 1$, see the following examples.

Example 1 Consider the graph $G = (V, E)$ with vertex set $V = \{1, \dots, k\} \cup \{a, b\}$ and $E = \{[i, j] \mid i, j \in \{1, \dots, k\}, i \neq j\} \cup \{[k, a], [a, b]\}$. The graph G is not a cograph, since there are induced P_4 's of the form $i - k - a - b$, $i \in \{1, \dots, k - 1\}$. On the other hand, the subgraph $H = (V, E \setminus \{[k, a]\})$ has two connected components, one is isomorphic to the complete graph K_k on k vertices and the other to the complete graph K_2 . Hence, H is a cograph. Therefore, G has a cograph 2-partition $\{E \setminus \{[k, a]\}, \{[k, a]\}\}$, independent from k and thus, independent from the maximum degree $\Delta = k$.

Example 2 Consider the $2n$ -dimensional hypercube $Q_{2n} = (V, E)$ with maximum degree $2n$. We will show that this hypercube has a coarsest cograph n -partition $\Pi = \{E_1, \dots, E_n\}$, which implies that for any optimal cograph k -decomposition of Q_{2n} we have $k \leq \Delta/2$.

We construct now a cograph n -partition of Q_{2n} . Note, $Q_{2n} = \square_{i=1}^{2n} K_2 = \square_{i=1}^n (K_2 \square K_2) = \square_{i=1}^n Q_2$. In order to avoid ambiguity, we write $\square_{i=1}^n Q_2$ as $\square_{i=1}^n H_i$, $H_i \simeq Q_2$ and assume that Q_2 has edges $[0, 1]$, $[1, 2]$, $[2, 3]$, $[3, 0]$. The cograph n -partition of Q_{2n} is defined as $\Pi = \{E_1, \dots, E_n\}$, where $E_i = \cup_{v \in V} E(H_i^v)$. In other words, the edge set of all H_i -layers in Q_{2n} constitute a single class E_i in the partition for each i . Therefore, the subgraph $G = (V, E_i)$ consists of n connected components, each component is isomorphic to the square Q_2 . Hence, $G_i = (V, E_i)$ is a cograph.

Assume for contradiction that $\Pi = \{E_1, \dots, E_n\}$ is not a coarsest partition. Then there are distinct classes E_i , $i \in I \subseteq \{1, \dots, n\}$ such that $G_I = (V, \cup_{i \in I} E_i)$ is a cograph. W.l.o.g. assume that $1, 2 \in I$ and let $v = (0, \dots, 0) \in V$. Then, the subgraph $H_1^v \cup H_2^v \subseteq Q_{2n}$ contains a path P_4 with edges $[x, v] \in E(H_1^v)$ and $[v, a], [a, b] \in E(H_2^v)$, where $x = (1, 0, \dots, 0)$, $a = (0, 1, 0, \dots, 0)$ and $b = (0, 2, 0, \dots, 0)$. By definition of the Cartesian product, there are no edges connecting x with a or b or v with b in Q_{2n} and thus, this path P_4 is induced. As this holds for all subgraphs $H_i^v \cup H_j^v$ ($i, j \in I$ distinct) and thus, in particular for the graph G_I we can conclude that classes of Π cannot be combined. Hence Π is a coarsest cograph n -partition.

Because of the results of computer-aided search for $n - 1$ -partitions and decompositions of hypercubes Q_{2n} we are led to the following conjecture:

Conjecture 2 Let $k \in \mathbb{N}$ and $k > 1$. Then the $2k$ -cube has no cograph $k - 1$ -decomposition, i.e., the proposed k -partition of the hypercube Q_{2k} in Example 2 is also optimal.

The proof of the latter hypothesis would immediately verify the next conjecture.

Conjecture 3 For every $k \in \mathbb{N}$ there is a graph that has an *optimal* cograph k -decomposition.

Proving the last conjecture appears to be difficult. We wish to point out that there is a close relationship to the problem of finding pattern avoiding words, see e.g. [5, 7, 30, 29, 3, 2]: Consider a graph $G = (V, E)$ and an ordered list (e_1, \dots, e_m) of the edges $e_i \in E$. We can associate to this list (e_1, \dots, e_m) a word $w = (w_1, \dots, w_m)$. By way of example, assume that we want to find a valid cograph 2-decomposition $\{E_1, E_2\}$ of G and that G contains an induced P_4 consisting of the edges e_i, e_j, e_k . Hence, one has to avoid assignments of the edges e_i, e_j, e_k to the single set E_1 , resp., E_2 . The latter is equivalent to find a binary word (w_1, \dots, w_m) such that $(w_i, w_j, w_k) \neq (X, X, X)$, $X \in \{0, 1\}$ for each of those induced P_4 's. The latter can easily be generalized to find pattern avoiding words over an alphabet $\{1, \dots, k\}$ to get a valid k -decomposition. However, to the authors knowledge, results concerning the counting of k -ary words, avoiding forbidden patterns and thus, verifying if there is any such word (or equivalently a k -decomposition) are basically known for scenarios like: If $(p_1, \dots, p_l) \in \{1, \dots, k\}^l$ (often $l < 3$), then none of the words w that contain

a subword $(w_{i_1}, \dots, w_{i_l}) = (p_1, \dots, p_l)$ with $i_{j+1} = i_j + 1$ (consecutive letter positions) or $i_j < i_k$ whenever $j < k$ (order-isomorphic letter positions) is allowed. However, such findings are too restrictive to our problem, since we are looking for words, that have only on a few, but fixed positions of non-allowed patterns. Nevertheless, we assume that results concerning the recognition of pattern avoiding words might offer an avenue to solve the latter conjectures.

5.1 Computational Complexity

In the following, we will prove the NP-completeness of COTREE 2-REPRESENTATION and COTREE 2-DECOMPOSITION. Additionally, these results allow to show that the problem of determining whether there is cograph 2-partition is NP-complete, as well.

We start with two lemmata concerning cograph 2-decompositions of the graphs shown in Fig. 5 and 6.

Lemma 1 *For the literal and extended literal graph in Figure 5 every cograph 2-decomposition is a uniquely determined cograph 2-partition.*

In particular, in every cograph 2-partition $\{E_1, E_2\}$ of the extended literal graph, the edges of the triangle $(0, 1, 2)$ must be entirely contained in one E_i and the pending edge $[6, 9]$ must be in the same edge set E_i as the edges of the triangle. Furthermore, the edges $[9, 10]$ and $[9, 11]$ must be contained in E_j , $i \neq j$.

Proof It is easy to verify that the given cograph 2-partition $\{E_1, E_2\}$ in Fig. 5 fulfills the conditions and is correct, since $G_1 = (V, E_1)$ and $G_2 = (V, E_2)$ do not contain induced P_4 's and are, thus, cographs. We have to show that it is also unique.

Assume that there is another cograph 2-decomposition $\{F_1, F_2\}$. Note, for any cograph 2-decomposition $\{F_1, F_2\}$ it must hold that two incident edges in the triangle $(0, 1, 2)$ are contained in one of the sets F_1 or F_2 . W.l.o.g. assume that $[0, 1], [0, 2] \in F_1$.

Assume first that $[1, 2] \notin F_1$. In this case, because of the paths $P_4 = 6 - 2 - 0 - 1$ and $P_4 = 2 - 0 - 1 - 5$ it must hold that $[2, 6], [1, 5] \notin F_1$ and thus, $[2, 6], [1, 5] \in F_2$. However, in this case and due to the paths $P_4 = 6 - 2 - 1 - 4$ and $2 - 0 - 1 - 4$ the edge $[1, 4]$ can neither be contained in F_1 nor in F_2 , a contradiction. Hence, $[1, 2] \in F_1$.

Note, the square S_{1256} induced by vertices 1, 2, 5, 6 cannot have all edges in F_1 , as otherwise the subgraph (V, F_1) would contain the induced $P_4 = 6 - 5 - 1 - 0$. Assume that $[1, 5] \in F_1$. As not all edges S_{1256} are contained in F_1 , at least one of the edges $[5, 6]$ and $[2, 6]$ must be contained in F_2 . If only one of the edges $[5, 6]$, resp., $[2, 6]$ is contained in F_2 , we immediately obtain the induced $P_4 = 6 - 2 - 1 - 5$, resp., $6 - 5 - 1 - 2$ in (V, F_1) and therefore, both edges $[5, 6]$ and $[2, 6]$ must be contained in F_2 . But then the edge $[2, 7]$ can neither be contained in F_1 (due to the induced $P_4 = 5 - 1 - 2 - 7$) nor in F_2 (due to the induced $P_4 = 5 - 6 - 2 - 7$), a contradiction. Hence, $[1, 5] \notin F_1$

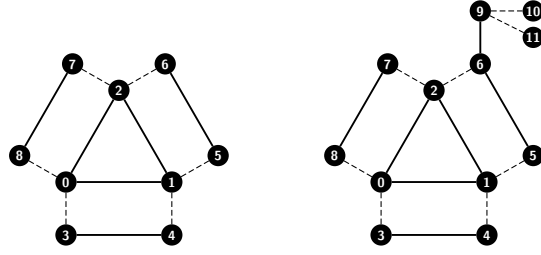


Fig. 5 Left the *literal graph* and right the *extended literal graph* with unique corresponding cograph 2-partition (indicated by dashed and bold-lined edges) is shown.

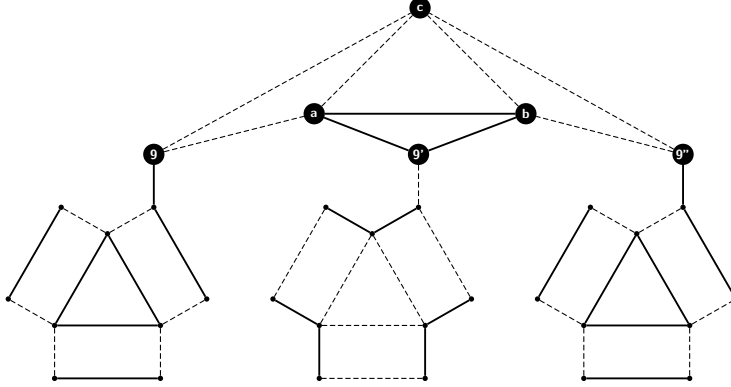


Fig. 6 Shown is a *clause gadget* which consists of a triangle (a, b, c) and three extended literal graphs (as shown in Fig. 5) with edges attached to (a, b, c) . A corresponding cograph 2-partition is indicated by dashed and bold-line edges.

and thus, $[1, 5] \in F_2$ for any 2-decomposition. By analogous arguments and due to symmetry, all edges $[0, 3]$, $[0, 8]$, $[1, 4]$, $[2, 6]$, $[2, 7]$ are contained in F_2 , but not in F_1 .

Moreover, due to the induced $P_4 = 7 - 2 - 6 - 5$ and since $[2, 6], [2, 7] \in F_2$, the edge $[5, 6]$ must be in F_1 and not in F_2 . By analogous arguments and due to symmetry, it holds that $[3, 4], [7, 8] \in F_1$ and $[3, 4], [7, 8] \notin F_2$. Finally, none of the edges of the triangle $(0, 1, 2)$ can be contained in F_2 , as otherwise, we obtain an induced P_4 in (V, F_2) . Taken together, any 2-decomposition of the literal graph must be a partition and is unique.

Consider now the extended literal graph in Figure 5. As this graph contains the literal graph as induced subgraph, the unique 2-partition of the underlying literal graph is determined as by the preceding construction. Due to the path $P_4 = 7 - 2 - 6 - 9$ with $[2, 6], [2, 7] \in F_2$ we can conclude that $[6, 9] \notin F_2$ and thus $[6, 9] \in F_1$. Since there are induced paths $P_4 = 5 - 6 - 9 - y$, $y = 10, 11$ with $[5, 6], [6, 9] \in F_1$ we obtain that $[9, 10], [9, 11] \notin F_1$ and thus, $[9, 10], [9, 11] \in F_2$ for any 2-decomposition (which is in fact a 2-partition) of the extended literal graph, as claimed. \square

Lemma 2 *Given the clause gadget in Fig. 6.*

For any cograph 2-decomposition, all edges of exactly two of the triangles in the underlying three extended literal graphs must be contained in one E_i and not in E_j , while the edges of the triangle of one extended literal graph must be in E_j and not in E_i , $i \neq j$.

Furthermore, for each cograph 2-decomposition exactly two of the edges e, e' of the triangle (a, b, c) must be in one E_i while the other edge f is in E_j but not in E_i , $j \neq i$. The cograph 2-decomposition can be chosen so that in addition $e, e' \notin E_j$, resulting in a cograph 2-partition of the clause gadget.

Proof It is easy to verify that the given cograph 2-partition in Fig. 6 fulfills the conditions and is correct, as $G_1 = (V, E_1)$ and $G_2 = (V, E_2)$ are cographs.

As the clause gadget contains the literal graph as induced subgraph, the unique 2-partition of the underlying literal graph is determined as by the construction given in Lemma 1. Thus, each edge of the triangle in each underlying literal graph is contained in either one of the sets E_1 or E_2 . Assume that edges of the triangles in the three literal gadgets are *all* contained in the same set, say E_1 . Then, Lemma 1 implies that $[9, a], [9, c], [9', a], [9', b], [9'', b], [9'', c] \in E_2$ and none of them is contained in E_1 . Since there are induced P_4 's: $9 - a - b - 9''$, $9' - a - c - 9''$ and $9 - c - b - 9'$, the edges $[a, b], [a, c], [b, c]$ cannot be contained in E_2 , and thus must be in E_1 . However, this is not possible, since then we would have the induced paths $P_4 = 9 - a - 9' - b$ in the subgraph (V, E_2) a contradiction. Thus, the edges of the triangle of exactly one literal gadget must be contained in a different set E_i than the edges of the other triangles in the other two literal gadgets. W.l.o.g. assume that the 2-decomposition of the underlying literal gadgets is given as in Fig. 6. and identify bold-lined edges with E_1 and dashed edges with E_2 .

It remains to show that this 2-decomposition of the underlying three literal gadgets determines which of the edges of triangle (a, b, c) are contained in which of the sets E_1 and E_2 . Due to the induced path $9 - a - b - 9''$ and since $[9, a], [9'', b] \in E_2$, the edge $[a, b]$ cannot be contained in E_2 and thus, is contained in E_1 . Moreover, if $[b, c] \notin E_2$, then there is an induced path $P_4 = b - 9'' - c - 9$ in the subgraph (V, E_2) , a contradiction. Hence, $[b, c] \in E_2$ and by analogous arguments, $[a, c] \in E_2$. If $[b, c] \notin E_1$ and $[a, c] \notin E_1$, then we obtain a cograph 2-partition. However, it can easily be verified that there is still a degree of freedom and $[a, c], [b, c] \in E_1$ is allowed for a valid cograph 2-decomposition. \square

We are now in the position to prove the NP-completeness of COTREE 2-REPRESENTATION and COTREE 2-DECOMPOSITION by reduction from the following problem.

Problem MONOTONE NAE 3-SAT

- Input:* Given a set U of Boolean variables and a set of clauses $\psi = \{C_1, \dots, C_m\}$ over U such that for all $i = 1, \dots, m$ it holds that $|C_i| = 3$ and C_i contains no negated variables.
- Question:* Is there a truth assignment to ψ such that in each C_i not all three literals are set to true?

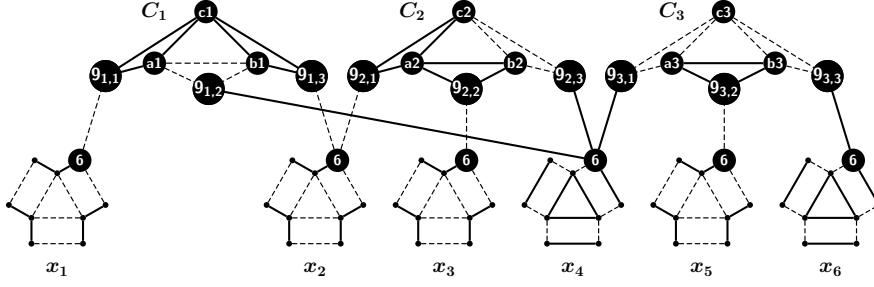


Fig. 7 Shown is the graph Ψ as constructed in the proof of Theorem 10. In particular, Ψ reflects the NAE 3-SAT formula $\psi = \{C_1, C_2, C_3\}$ with clauses $C_1 = (x_1, x_4, x_2)$, $C_2 = (x_2, x_3, x_4)$ and $C_3 = (x_4, x_5, x_6)$. Different literals obtain the same truth assignment true or false, whenever the edges of the triangle in their corresponding literal gadget are contained in the same set E_i of the cograph 2-partition, highlighted by dashed and bold-lined edges.

Theorem 9 ([31,28]) *MONOTONE NAE 3-SAT is NP-complete.*

Theorem 10 *COGRAPH 2-DECOMPOSITION, and thus, COTREE 2-REPRESENTATION is NP-complete.*

Proof Given a graph $G = (V, E)$ and cograph 2-decomposition $\{E_1, E_2\}$, one can verify in linear time whether (V, E_i) is a cograph [8]. Hence, COGRAPH 2-PARTITION \in NP.

We will show by reduction from MONOTONE NAE 3-SAT that COGRAPH 2-DECOMPOSITION is NP-hard. Let $\psi = (C_1, \dots, C_m)$ be an arbitrary instance of MONOTONE NAE 3-SAT. Each clause C_i is identified with a triangle (a_i, b_i, c_i) . Each variable x_j is identified with a literal graph as shown in Fig. 5 (left) and different variables are identified with different literal graphs. Let $C_i = (x_{i_1}, x_{i_2}, x_{i_3})$ and G_{i_1} , G_{i_2} and G_{i_3} the respective literal graphs. Then, we extend each literal graph G_{i_j} by adding an edge $[6, 9_{i,j}]$. Moreover, we add to G_{i_1} the edges $[9_{i,1}, a_i], [9_{i,1}, c_i]$, to G_{i_2} the edges $[9_{i,2}, a_i], [9_{i,2}, b_i]$, to G_{i_3} the edges $[9_{i,3}, c_i], [9_{i,3}, b_i]$. The latter construction connects each literal graph with the triangle (a_i, b_i, c_i) of the respective clause C_i in a unique way, see Fig. 6. We denote the clause gadgets by Ψ_i for each clause C_i . We repeat this construction for all clauses C_i of ψ resulting in the graph Ψ . An illustrative example is given in Fig. 7. Clearly, this reduction can be done in polynomial time in the number m of clauses.

We will show in the following that Ψ has a cograph 2-decomposition (resp., a cograph 2-partition) if and only if ψ has a truth assignment f .

Let $\psi = (C_1, \dots, C_m)$ have a truth assignment. Then in each clause C_i at least one of the literals $x_{i_1}, x_{i_2}, x_{i_3}$ is set to true and one to false. We assign all edges e of the triangle in the corresponding literal graph G_{i_j} to E_1 , if $f(x_{i_j}) = \text{true}$ and to E_2 , otherwise. Hence, each edge of exactly two of the triangles (one in G_{i_j} and one in $G_{i_{j'}}$) are contained in one E_r and not in E_s , while the edges of the other triangle in $G_{i_{j''}}$, $j'' \neq j, j'$ are contained in E_s and not in E_r , $r \neq s$, as needed for a possible valid cograph 2-decomposition (Lemma 2). We now apply the construction of a valid cograph 2-decomposition

(or cograph 2-partition) for each Ψ_i as given in Lemma 2, starting with the just created assignment of edges contained in the triangles in G_{i_j} , $G_{i_{j'}}$ and $G_{i_{j''}}$ to E_1 or E_2 . In this way, we obtain a valid cograph 2-decomposition (or cograph 2-partition) for each subgraph Ψ_i of Ψ . Thus, if there would be an induced P_4 in Ψ with all edges belonging to the same set E_r , then this P_4 can only have edges belonging to different clause gadgets Ψ_k, Ψ_l . By construction, such a P_4 can only exist along different clause gadgets Ψ_k and Ψ_l if C_k and C_l have a literal $x_i = x_{k_m} = x_{l_n}$ in common. In this case, Lemma 2 implies that the edges $[6, 9_{k,m}]$ and $[6, 9_{l,n}]$ in Ψ_i must belong to the same set E_r . Again by Lemma 2, the edges $[9_{k,m}, y]$ and $[9_{k,m}, y']$, $y, y' \in \{a_k, b_k, c_k\}$ as well as the edges $[9_{l,n}, y]$ and $[9_{l,n}, y']$, $y, y' \in \{a_l, b_l, c_l\}$ must be in a different set E_s than $[6, 9_{k,m}]$ and $[6, 9_{l,n}]$. Moreover, respective edges $[5, 6]$ in Ψ_k , as well as in Ψ_l (Fig. 5) must be in E_r , i.e., in the same set as $[6, 9_{k,m}]$ and $[6, 9_{l,n}]$. However, in none of the cases it is possible to find an induced P_4 with all edges in the same set E_r or E_s along different clause gadgets. Hence, we obtain a valid cograph 2-decomposition, resp., cograph 2-partition of Ψ .

Now assume that Ψ has a valid cograph 2-decomposition (or a cograph 2-partition). Any variable x_{i_j} contained in some clause $C_i = (x_{i_1}, x_{i_2}, x_{i_3})$ is identified with a literal graph G_{i_j} . Each clause C_i is, by construction, identified with exactly three literal graphs $G_{i_1}, G_{i_2}, G_{i_3}$, resulting in the clause gadget Ψ_i . Each literal graph G_{i_j} contains exactly one triangle t_j . Since Ψ_i is an induced subgraph of Ψ , we can apply Lemma 2 and conclude that for any cograph 2-decomposition (resp., cograph 2-partition) all edges of exactly two of three triangles t_1, t_2, t_3 are contained in one set E_r , but not in E_s , and all edges of the other triangle are contained in E_s , but not in E_r , $s \neq r$. Based on these triangles we define a truth assignment f to the corresponding literals: w.l.o.g. we set $f(x_i) = \text{true}$ if the edge $e \in t_i$ is contained in E_1 and $f(x_i) = \text{false}$ otherwise. By the latter arguments and Lemma 2, we can conclude that, given a valid cograph 2-partitioning, the so defined truth assignment f is a valid truth assignment of the Boolean formula ψ , since no three different literals in one clause obtain the same assignment and at least one of the variables is set to *true*. Thus, COGRAPH 2-DECOMPOSITION is NP-complete

Finally, because COGRAPH 2-DECOMPOSITION and COTREE 2-REPRESENTATION are equivalent problems, the NP-completeness of COTREE 2-REPRESENTATION follows. \square

As the proof of Theorem 10 allows us to use cograph 2-partitions in all proof steps, instead of cograph 2-decompositions, we can immediately infer the NP-completeness of the following problem for $k = 2$, as well.

Problem COGRAPH k -PARTITION

Input: Given a graph $G = (V, E)$ and an integer k .

Question: Is there a Cograph k -Partition of G ?

Theorem 11 COGRAPH 2-PARTITION is NP-complete.

As a direct consequence of the latter results, we obtain the following result.

Corollary 2 *Let G be a given graph that is not a cograph. The three optimization problems to find the least integer $k > 1$ so that there is a Cograph k -Partition, a Cograph k -Decomposition, or a Cotree k -Representation for the graph G , are NP-hard.*

5.2 Integer Linear Program

Let $G = (V, E)$ be a given graph with maximum degree Δ . We want to find a cograph- k -decomposition, resp., partition $\Pi = \{E_1, \dots, E_k\}$ for the least integer k . Theorem 8 implies that the least integer k is always less or equal to $\Delta + 1$.

We define binary variables E_{xy}^i for all $x, y \in V$ and $1 \leq i \leq \Delta + 1$ s.t. $E_{xy}^i = 1$ if and only if the edge $[x, y] \in E$ is contained in class E_i of Π . Moreover, we define the binary variables M^i with $1 \leq i \leq \Delta + 1$ so that $M^i = 1$ if and only if the class $E_i \in \Pi$ is non-empty in our construction. In other words, $\sum_{1 \leq i \leq \Delta+1} M^i$ will be the cardinality of Π .

In order to find the cograph decomposition, resp., partition Π of G having the fewest number of elements we need the following objective function.

$$\min \sum_{1 \leq i \leq \Delta+1} M^i \quad (8)$$

If we want to find a cograph-decomposition and hence, that each edge is contained in at least one class E_i of Π we need the next constraint.

$$\sum_{1 \leq i \leq \Delta+1} E_{xy}^i \geq 1 \text{ for all } [x, y] \in E. \quad (9)$$

In contrast, if we want to find a cograph-partition and hence, that each edge is contained in exactly one class E_i of Π we need this constraint.

$$\sum_{1 \leq i \leq \Delta+1} E_{xy}^i = 1 \text{ for all } [x, y] \in E. \quad (9')$$

Moreover, we must ensure that non-edges $[x, y] \notin E$ are not contained in any class of Π which is done with the next constraint.

$$\sum_{1 \leq i \leq \Delta+1} E_{xy}^i = 0 \text{ for all } [x, y] \notin E. \quad (10)$$

Whenever there is a class E_i containing an edge $[x, y] \in E$ and hence, if $E_{xy}^i = 1$ then we must set $M^i = 1$.

$$\sum_{x, y \in V} E_{xy}^i \leq |V|^2 M^i \text{ for all } 1 \leq i \leq \Delta + 1. \quad (11)$$

Finally we have to ensure that each subgraph $G_i = (V, E_i)$ is a cograph, and thus, does not contain induced P_4 's, which is achieved with the following constraint.

$$E_{xy}^i + E_{yu}^i + E_{uv}^i - E_{xu}^i - E_{xv}^i - E_{yv}^i \leq 2 \quad (12)$$

for all $1 \leq i \leq \Delta + 1$ and all ordered tuples (x, y, u, v) of distinct $x, y, u, v \in V$.

This ILP-formulation needs $O(\Delta|V|^2)$ variables and $O(|E| + \Delta + |V|^4)$ constraints.

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